



Società Chimica Italiana
Divisione di Chimica Fisica



Dipartimento di
Biotechnologie e Bioscienze



Dipartimento di
Chimica Fisica ed Electrochimica

XXXIX

congresso nazionale

Stresa

20 - 24 settembre 2010

design

Studio Luca Negri & Associati

stampa

Arti Grafiche Baratelli

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Lunedì 20 settembre 2010

10:00 – 13:00	Registrazione partecipanti
14:00 – 14:15	Apertura del Congresso

Sessione I

14:15 – 15:00	L1 – <u>Gregory D. Scholes</u> <i>Quantum coherence in photosynthetic light-harvesting: What it means for quantum biology</i>
15:00 – 15:15	O1 – <u>C. Puzzarini</u> , J. Gauss <i>Benchmarking Quantum Chemistry with Rotational Spectroscopy or Benchmarking Rotational Spectroscopy with Quantum Chemistry?</i>
15:15 – 15:30	O2 – <u>A. Marchetti</u> , V. Domenici, A. J. Pell, M. Lelli, M. Cifelli, A. Lesage, C. A. Veracini <i>New physical insights on deVries smectic liquid crystals by means of 2H- and 13C-NMR spectroscopy</i>
15:30 – 15:45	O3 – <u>E. Romano</u> , G. F. Cerofolini, D. Narducci, F. Corni, S. Frabboni, G. Ottaviani, R. Tonini <i>A tool for the spectroscopic investigation of hydrogen-silicon interaction</i>
15:45 – 16:00	O4 – <u>A. Marini</u> , A. Muñoz-Losa, B. Mennucci, A. Pucci, G. Ruggeri <i>Which strategy for molecular probe design? An answer from the integration of spectroscopy and Quantum Mechanical modeling</i>
16:00 – 16:30	<i>Pausa caffè</i>
16:30 – 16:45	O5 – <u>G. Brancato</u> , N. Rega, V. Barone <i>Structural and Vibrational analysis of XAFS spectroscopy by ab-initio molecular dynamics: Zn²⁺ in aqueous solution</i>
16:45 – 17:00	O6 – <u>B. Carlotti</u> , F. Elisei, A. Spalletti <i>Dynamics of the lowest excited singlet states of nitroaromatics investigated by time-resolved techniques</i>
17:00 – 17:15	O7 – <u>F. Puntoriero</u> , S. Campagna, J. Fortage, F. Tuyéras, P. Lainé <i>Photophysical properties of new polyaryl-bipyridinium containing - Ru(II) and Os(II) molecular dyads</i>

17:15 – 17:30	O8 – F. Carniato, <u>C. Bisio</u> , G. Gatti, G. Paul, L Bertinetti, S. Coluccia, L. Marchese <i>On the physico-chemical properties of hydrothermally stable luminescent MCM-41 nanoparticles</i>
17:30 – 19:00	Presentazione Poster Sessione 1 15 comunicazioni da 5'
19:00	<i>Cocktail di benvenuto</i>

Martedì 21 settembre 2010

Sessione II

9:00 – 9:45	L2 – <u>Fabrizio Santoro</u> <i>Computational Approach to Electronic Spectroscopy</i>
9:45 – 10:00	O9 – I. Russo Krauss, A. Merlino, A. Randazzo, C. Giancola, L. Mazzarella, <u>F. Sica</u> <i>High resolution X-ray structure of the complex of human alpha thrombin with a modified thrombin binding aptamer</i>
10:00 – 10:15	O10 – M. P. Costi, S. Ferrari, <u>G. Ponterini</u> <i>Physico-chemical tools in anticancer drug research: targeting human Thymidylate synthase with synthetic octapeptides</i>
10:15 – 10:30	O11 – <u>L. Petraccone</u> , J. Trent, C. Giancola, J. B. Chaires <i>Experimental and Computational Studies of Higher Order Human Telomeric Quadruplexes</i>
10:30 – 10:45	O12 – <u>G. Saladino</u> , S. Rendine, S. Pieraccini, M. Sironi <i>Modeling of peptides that mimic protein-protein interactions</i>
10:45 – 11:15	<i>Pausa caffè</i>
11:15 – 11:30	O13 – <u>R. Pogni</u> , R. Basosi <i>The catalytic cycle of versatile peroxidases: a EPR story</i>
11:30 – 11:45	O14 – <u>L. Ambrosone</u> <i>The dielectric response of non-spherical live cells in suspension</i>
11:45 – 12:00	O15 – <u>L. Giussani</u> , E. Fois, E. Gianotti, G. Tabacchi, A. Gamba, S. Coluccia <i>On how a water-solvated protein wets a silica surface</i>

12:00 – 12:15	O16 – <u>A. Salis</u> , D. F. Parsons, M. Bostrom, B. W. Ninham, M. Monduzzi <i>Specific Ion Effects at SBA-15 Mesoporous Silica solid/liquid Interface: Protein Adsorption and Surface Charge Density</i>
12:15 – 12:30	O17 – A. Ardu, C. Cannas, F. Orrù, <u>A. Musinu</u> , D. Peddis, G. Piccaluga <i>Hydrophilic magnetic nanostructures for biomedical applications</i>
12:30 – 14:00	<i>Pausa</i>

Sessione III

14:00 – 14:45	L3 – <u>Rodorigo Giorgi</u> <i>Nanotechnology for the restoration of art masterpieces</i>
14:45 – 15:00	O18 – <u>G. Poggi</u> , R. Giorgi, N. Toccafondi, P. Baglioni <i>Magnesium hydroxide nanoparticles for deacidification and inhibition of metal-gall ink corrosion of paper</i>
15:00 – 15:15	O19 – M. Baglioni, J. Teixeira, R. Giorgi, M. Bonini, P. Baglioni, <u>D. Berti</u> <i>NanoStructured Cleaning Systems for the Removal of Organic Polymers From Wall Paintings – A SANS study</i>
15:15 – 15:30	O20 – <u>E. Collina</u> , M. Lasagni, M. Ferri, C. Acaia, D. Pitea <i>Sewage sludge characterization for mass and energy balances in an integrated drying and combustion system</i>
15:30 – 16:30	<i>“La conoscenza scientifica non può essere fredda” ricordando Enzo Tiezzi</i>
16:30 – 17:00	<i>Pausa caffè</i>
17:00 – 18:15	Sessione Poster 1: P1 – P58

18:15 – 19:45	<p>Tavola Rotonda</p> <p><i>In partibus infidelium ovvero l'insegnamento della Chimica Fisica nei corsi di studio non chimici</i></p> <p>Coordina: Stefania Milioto</p>
	<p>Marilena Carnasciali <i>La presenza della Chimica Fisica nei corsi di studio non chimici</i></p> <p>Michele A. Floriano <i>La Chimica Fisica nelle Scienze Ambientali</i></p> <p>Mariano Venanzi <i>La Chimica Fisica nelle Scienze Biologiche</i></p>

Mercoledì 22 settembre 2010

Sessione IV

9:00 – 9:45	<p>L4 – Alessandro Vergara <i>Raman-assisted X-ray biocrystallography. Applications to metal proteins</i></p>
9:45 – 10:00	<p>O21 – M. Caruso, E. Gatto, R. Lettieri, D. Monti, A. Porchetta, D. Roversi, E. Placidi, <u>M. Venanzi</u> <i>Soft meets hard. Spectroscopic and electrochemical investigation of organic films supported on inorganic substrates</i></p>
10:00 – 10:15	<p>O22 – <u>G. Lazzara</u>, B. Nyström, G. Olofsson, K. Schillén <i>Threading and de-threading of cyclodextrin in a thermosensitive cationic block copolymer in water and at the silica/water interface</i></p>
10:15 – 10:30	<p>O23 – <u>C. Tedesco</u>, L. Erra, V. Cipolletti, G. Vaughan, M. Brunelli, C. Gaeta, P. Neri <i>Host-guest interactions in a calixarene-based nanoporous material</i></p>
10:30 – 10:45	<p>O24 – <u>S. Bettini</u>, S. Bonsegna, R. Pagano, A. Zacheo, V. Vergaro, G. Giovinazzo, G. Caminati, S. Leporatti, L. Valli, A. Santino <i>Plant oil bodies as novel carriers to deliver lipophilic molecules</i></p>
10:45 – 11:15	<p><i>Pausa caffè</i></p>

11:15 – 12:45	Presentazione Poster Sessione 2 15 comunicazioni da 5'
12:45 – 14:30	<i>Pausa</i>

Sessione V

14:30 – 15:15	L5 – <u>Niyazi Serdar Sariciftci</u> <i>Organic Nanostructures for Solar Energy Conversion: From Photovoltaic Electricity to Synthetic Fuels using CO₂ Recycling</i>
15:15 – 15:30	O25 – <u>G. L. Chiarello</u>, E. Selli <i>Hydrogen production by photo-steam reforming of methanol: effect of noble metals-deposition on TiO₂</i>
15:30 – 15:45	O26 – <u>P. Canton</u>, A. Benedetti, T. Montini, A. Hameed, V. Gombac, P. Fornasiero <i>Structural characterization and Photocatalytic Activity Correlation of Bi₂O₃/Bi₂O_{4-x} Nanocomposite</i>
15:45 – 16:00	O27 – F. Petronella, E. Fanizza, M. Striccoli, G. Mascolo, S. Diomede, V. Locaputo, A. Agostiano, M. L. Curri, <u>R. Comparelli</u> <i>Photocatalytic activity of metal/semiconductor based nanosized catalysts under UV irradiation</i>
16:00 – 16:30	<i>Pausa caffè</i>
16:30 – 16:45	O28 – S. Cataldo, S. Fabiano, C. Sartorio, S. Patané, <u>B. Pignataro</u> <i>Engineering 3D nanoscale order in molecular thin films for organic photovoltaics</i>
16:45 – 17:00	O29 – <u>C. Milanese</u>, A. Girella, S. Garroni, G. Mulas, E. Napolitano, S. Suriñach, M.D. Baró, A. Marini <i>Hydrogen sorption properties of the NaBH₄ – MgH₂ system</i>
17:00 – 17:15	O30 – <u>S. Morandi</u>, F. Prinetto, G. Ghiotti, L. Castoldi, I. Nova, L. Lietti <i>FT-IR study of the water effect on surface species formed during the operation of Nox storage-reduction catalysts</i>

17:15 – 17:30	O31 – <u>C. Tealdi</u> , P. Mustarelli, M. S. Islam <i>Layered LaSrGa3O7-Based Oxide-Ion Conductors: The Importance of Cooperative Transport Mechanisms and Flexible Structures</i>
17:30 – 17:45	O32 – <u>A. Minguzzi</u> , D. Battistel, C. Locatelli, J. Rodriguez Lopez, A. Vertova, S. Daniele, S. Rondinini, A. J. Bard <i>Recent developments in the rapid screening of electro-catalysts and a new representation of their activity</i>
17:45 – 19:15	Assemblea della Divisione di Chimica Fisica

Giovedì 23 settembre 2010

Sessione VI

9:00 – 9:45	L6 – <u>Marie-Paule Pileni</u> <i>Self assembly of nanocrystals: a new chance for the future</i>
9:45 – 10:00	O33 – <u>A. Triolo</u> , O. Russina, R. Caminiti <i>Mesoscopic organization in ionic liquids: structural and dynamic implications</i>
10:00 – 10:15	O34 – V. Barone, J. Bloino, I. Cacelli, A. Ferretti, S. Monti, A. Pedone, <u>G. Prampolini</u> <i>Accurate Force Fields for Soft Matter Computer Simulations</i>
10:15 – 10:30	O35 – <u>A. Forni</u> <i>Unravelling the nature of halogen bonding: experimental and theoretical studies</i>
10:30 – 10:45	O36 – <u>E. Chiessi</u> , G. Paradossi, A. Lonardi <i>Toward Modeling Thermoresponsive Polymer Networks: A Molecular Dynamics Simulation Study of N-Isopropyl Acrylamide Co-Oligomers</i>
10:45 – 11:15	<i>Pausa caffè</i>
11:15 – 11:30	O37 – A. Pizzirusso, M. Savini, L. Muccioli, <u>C. Zannoni</u> <i>A molecular dynamics investigation of the liquid-crystalline phases of the sexithiophene</i>
11:30 – 11:45	O38 – <u>G. Tabacchi</u> , Ettore Fois, Davide Barreca, Alberto Gasparotto, Eugenio Tondello <i>Molecular activation on hot-surfaces by first principles</i>

11:45 – 12:00	O39 – P Tempesti, <u>M Bonini</u> , F Ridi, P Baglioni <i>Magnetic Nanoparticles embedded within polystyrene beads: nano-composite materials for oil-recovery applications</i>
12:00 – 12:15	O40 – <u>C. Artini</u> , G.A. Costa, R. Masini <i>Structural studies of rare earths mixed oxides</i>
12:15 – 14:00	<i>Pausa</i> <i>Assemblea Generale S.C.I. 13:00 – 15:00</i>
14:00 – 15:15	Sessione Poster 2: P59 – P116
15:15 – 15:30	O41 – <u>C. Cappelli</u> <i>A Time-Independent Approach To Two-Dimensional Infrared Spectra (2D-IR) Of Molecules In Solution: Which Role for Continuum Solvation Models?</i>
15:30 – 15:45	O42 – <u>R. Dovesi</u> , R.Orlando, B. Civalleri, L. Maschio <i>Quantum mechanical simulation of the properties of crystalline solids with the CRYSTAL09 and CRYSCOR periodic codes</i>
15:45 – 16:00	O43 – <u>A. Girlando</u> , M. Masino, I. Bilotti, A. Brillante, R. G. Della Valle, E. Venuti <i>Peierls coupling in molecular crystals</i>
16:00 – 16:30	<i>Pausa caffè</i>
16:30 – 16:45	O44 – <u>E. Bodo</u> , R. Caminiti <i>Atomistic Simulation of Ionic Liquids: Dissecting Their Local Structure with Combined Experimental and Theoretical Determinations</i>
16:45 – 17:00	O45 – <u>S. Casolo</u> , R. Martinazzo, G.F. Tantardini <i>Electronic structure of substitutional defects superlattices in graphene</i>
17:00 – 17:15	O46 – <u>S Rampino</u> , G Ferraro, A Laganà, G. G. Balint-Kurti <i>Diatomic eigenvalue problem and wavepacket propagation for collinear H + H₂ using non orthogonal coordinates: the Bond Order formulation</i>
17:15	Visita alle Isole Borromee
20:00	Cena sociale

Venerdì 24 settembre 2010

Sessione VII

9:30 – 11:00	Tavola Rotonda a cura di Maurizio Casarin
11:00 – 11:15	Chiusura Congresso
11:45	<i>Assemblea della costituenda Divisione di Chimica Teorica e Computazionale</i>

Sessione poster 1

Martedì 21 settembre 2010

16:30 – 17:45

P1 - <u>A. Naldoni</u> , C. Pirola, C. L. Bianchi, K. S. Suslick <i>Silica-directed Growth of Anatase TiO₂ Hierarchical Hollow MicroSpheres</i>
P2 – <u>G. Giancane</u> , A. Ruland, V. Sgobba, D. Manno, A. Serra, G. M. Farinola, O. Hassan Omar, D. M. Guldi, L. Valli <i>Langmuir Blodgett films of aligned single wall carbon nanotubes. Morphological and photoelectrochemical studies</i>
P3 – <u>C. Montis</u> , S. Milani, P. Baglioni <i>Anionic Liposomes and DNA: Molecular Recognition and Reentrant Condensation</i>
P4 – T. H. Ngo, F. Puntoriero, <u>F. Nastasi</u> , K. Robeyns, L. Van Meervelt, S. Campagna, W. Dehaena, W. Maes <i>Photophysical exploration of meso-pyrimidinyl-substituted corroles and corroles-porphyrins supramolecular system</i>
P5 – <u>G. La Ganga</u> , F. Puntoriero, S. Campagna, A. Sartorel, M. Carraro, G. Scorrano, M. Bonchio <i>Photo-induced water oxidation with tetranuclear Ru(II) dendrimer as sensitizer</i>
P6 – P. Cavigli, <u>F. Gambinossi</u> , P. Baglioni, G. Caminati <i>Phosphorescent Organic Light Emitting Diodes of PVK-Iridium complexes in LB nanoassemblies</i>
P7 – <u>F. Lipparini</u> , B. Mennucci, E. Cancès, G. Scalmani, M. Caricato, M. J. Frisch <i>A variational formulation of the Polarizable Continuum Model</i>
P8 – C. Deiana, E. Fois, S. Coluccia, <u>G. Martra</u> <i>Surface structure of TiO₂ nanoparticles: focus on coordinative defective sites and related hydroxy groups</i>
P9 – P. Iliade, G. Berlier, <u>S. Coluccia</u> <i>Influence of the preparation method on the properties of hybrid organosilica NH₂-MCM-41</i>
P10 – <u>A. Merlino</u> , I. Russo Krauss, I. Castellano, E. De Vendittis, B. Rossi, M. Conte, A. Vergara, F. Sica <i>Structure, stability and dynamic properties and of cold-adapted iron superoxide dismutases in comparison with mesophilic homologues</i>

<p>P11 - <u>F. Spadavecchia</u>, S. Ardizzone, G. Cappelletti, L. Falciola, M. Leoni, P. Scardi <i>N-doped TiO₂ semiconductor nanoparticles. Bulk, surface and electrochemical features</i></p>
<p>P12 - <u>G. Barone</u>, I. Duro, D. Mastrangelo, R. Montella, A. Riccio, L. Varriale <i>Air pollution modeling: A project for the Campania Region Board</i></p>
<p>P13 - <u>G. Barone</u>, E. Chianese <i>Methane Hydrates: Resource or Climatic Threat? Stability of Natural Gases Hydrates and Exploitation Perspectives</i></p>
<p>P14 – <u>J. Scaranto</u>, S. Giorgianni <i>Infrared spectra and first principles simulations of CH₂FBr adsorbed on TiO₂</i></p>
<p>P15 - <u>O. Buchneva</u>, I. Rossetti, C. Oliva, M. Scavini, M. Allieta <i>Effective Ag doping and resistance to sulphur poisoning of La-Mn perovskites for the catalytic flameless combustion of methane</i></p>
<p>P16 - F. Gambinossi, M. Banchelli, D. Berti, P. Baglioni, <u>G. Caminati</u> <i>Sequential adsorption of amphiphilic DNA onto Supported Phospholipid Bilayers: a ‘Tetris-like’ scenario</i></p>
<p>P17 - <u>S. Samanipour</u>, T. Cecchi, P. Passamonti <i>Lycopene extraction kinetic model</i></p>
<p>P18 – <u>F. Ridi</u>, F. Cottone, M. Bonini, P. Baglioni <i>Study of interactions between a cellulosic polymer and polycarboxylate superplasticizers</i></p>
<p>P19 - G. Campiani, S. Butini, C. Bonechi, A. Donati, <u>C. Rossi</u> <i>Strategies to Potential Anticancer Agents Functionally Mimicking Activity of Nur-77 on Bcl-2: NMR studies of new oligopeptide PEP2</i></p>
<p>P20 - A. Puglisi, S. Mondini, A. M. Ferretti, N. Santo, M. Gemmi, <u>A. Ponti</u> <i>α-MnS and MnO Nanocrystals: Synthesis, Shape & Texture</i></p>
<p>P21 – <u>A. Pietropolli Charmet</u>, P. Stoppa, N. Tasinato, A. Baldan, S. Giorgianni, A. Gambi <i>Infrared spectra, integrated band intensities and ab initio calculations of CHBrF₂</i></p>
<p>P22 - <u>M. Ceotto</u>, D. Dell'Angelo, G. F. Tantardini <i>Multiple coherent states semiclassical representation for first principles molecular dynamics and dipole absorption spectra calculations of lateral interactions for CO on Cu(100)</i></p>

<p>P23 – F. Sannicolò, G. Rampinini, L. Colella, T. Benincori, S. Rizzo, W. Kutner, K. Noworyta, V. Bonometti, <u>P. Mussini</u> <i>Inherently chiral thiophene-based monomers: redox properties and electropolymerization</i></p>
<p>P24 – <u>E. Fois</u>, G. Tabacchi, G. Calzaferri <i>Water effects on dye-zeolite composite</i></p>
<p>P25 - K. Daasbjerg, S. U. Pedersen, V. De Renzi, N. Florini, F. Parenti, C. A. Bortolotti, D. Vanossi, <u>C. Fontanesi</u> <i>On the Electroreduction Mechanism of Iodonium Salts on Glassy Carbon Electrodes</i></p>
<p>P26 – <u>M. Magarelli</u>, P. Passamonti, A. Santaballa, M. Canle <i>Photodegradation of modified sepia melanin (sepia officinalis)</i></p>
<p>P27 - N. Faginas Lago, M. Albertí, A. Laganà <i>NMA in aqueous solution with intermolecular potentials</i></p>
<p>P28 – S. Murgia, S. Lampis, P. Hiwale, <u>M. Monduzzi</u> <i>Nanostructures for innovative drug delivery</i></p>
<p>P29 - M. Altomare, E. Fanizza, M. Corricelli, M. Striccoli, A. Agostiano, M.L. Curri <i>Luminescent semiconductor nanocrystal on micro-contact printing patterned surfaces</i></p>
<p>P30 – I. Meazzini, <u>M. Bonini</u>, P. Baglioni <i>Magnetic Nanoparticles and click-chemistry: a viable approach to functional nano-composite materials</i></p>
<p>P31 – <u>S. Ristori</u>, E. Di Cola, C. Lunghi, B. Richichi, C. Nativi <i>Structural study of liposomes loaded with a GM3 lactone analog for the targeting of tumor epitopes</i></p>
<p>P32 – E. Dilena, P. Mustarelli, <u>E. Quartarone</u>, A. Magistris, S. Angioni, P.P. Righetti <i>New oxy-PBI membranes as electrolytes for polymer fuel cells</i></p>
<p>P33 – L. Formaro, I. Galbiati, <u>M. Longhi</u>, C. Bianchi, E. Ragg <i>Platinum-free electrocatalysts for Oxygen Reduction Reaction in PEMFC from templated mixtures of sugarnitrogen bases</i></p>
<p>P34 – Ivana Finelli, Shivkumar Ghugare, Ester Chiessi, <u>Gaio Paradossi</u> <i>Soft Matter for Biomedicine: two case studies</i></p>
<p>P35 – <u>S. Rendine</u>, G. Saladino, S. Pieraccini, M. Sironi <i>In silico design of peptides inhibiting protein-protein interactions</i></p>
<p>P36 – E. Vittorino, G. Giancane, <u>S. Bettini</u>, L. Valli, S. Sortino <i>Simultaneous generation of nitric oxide and singlet oxygen from multilayer films of an organic dyad</i></p>

<p>P37 - M. Alderighi, C. Duce, <u>L. Ghezzi</u>, M. R. Tiné, R. Solaro <i>Calorimetric investigation of the RWDW oligopeptide self-assembly process</i></p>
<p>P38 - M. Caruso, E. Placidi, E. Gatto, C. Mazzuca, L. Stella, A. Palleschi, G. Bocchinfuso, F. Formaggio, C. Toniolo, <u>M. Venanzi</u> <i>Optical spectroscopy and conformational analysis of peptide aggregates: the role of aromatic interactions and conformational flexibility</i></p>
<p>P39 - <u>F. Martelli</u>, I. Burghardt, G. F. Tantardini, R. Martinazzo <i>A Model to Study Exciton Energy Transfer in Linear Chain Systems</i></p>
<p>P40 - <u>R. Martinazzo</u>, S. Casolo, G. F. Tantardini <i>Symmetry-induced bandgap opening in graphene superlattices</i></p>
<p>P41 - R. De Lisi, G. Giammona, G. Lazzara, <u>S. Milioto</u> <i>Solubilization of oils in aqueous solution of star-like block copolymer with thermo- and pH-sensitive features</i></p>
<p>P42 - G. Cavallaro, R. De Lisi, G. Lazzara, <u>S. Milioto</u> <i>Bionanocomposites Based on Pectins and Halloysite Nanotubes: from the Structure to the Properties</i></p>
<p>P43 - <u>C. Tealdi</u>, G. L. Chiarello, E. Quartarone, P. Mustarelli, E. Selli <i>TiO₂ photoelectrodes prepared by RF-Magnetron Sputtering: effect of thickness and deposition temperature on the separate hydrogen and oxygen evolution from water splitting</i></p>
<p>P44 - <u>V. Spampinato</u>, N. Tuccitto, N. Giambianco, S. Quici, E. Defrancq, A. Torrisi, A. Licciardello, G. Marletta <i>Surface engineering by metal-complex supramolecular coordination</i></p>
<p>P45 - <u>M. Altomare</u>, G. L. Chiarello, A. Costa, M. Guarino, E. Selli <i>Photocatalytic abatement of nitrogen content in waste waters</i></p>
<p>P46 - <u>E. Collini</u>, F. Todescato, C. Ferrante, R. Bozio, G. D. Scholes <i>Energy Transfer across metal films mediated by Surface Plasmon Polaritons: a time-resolved fluorescence study</i></p>
<p>P47 - M. C. Arroyo, P. Baglioni, D. Berti, <u>E. Fratini</u>, R. Giorgi <i>Ionic liquid/Brij 30/nonane microemulsions: Characterization and applications</i></p>
<p>P48 - R. Giorgi, <u>L. Bernini</u>, F. Ridi, P. Baglioni <i>Mesoamerican mural paintings. Physico-chemical characterization of natural exudate gums</i></p>
<p>P49 - R. Giorgi, <u>L. Bernini</u>, P. Baglioni <i>Mesoamerican mural paintings. Physico-chemical characterization of materials and application of calcium hydroxide nanoparticles for consolidation</i></p>

<p>P50 – I. Miglioli, A. Arcioni, C. Bacchiocchi, R. Berardi, L. Muccioli, <u>A. Pizzirusso</u>, D. Summa, A. Kohlmeier, M. G. Tamba, G. H. Mehlb, C. Zannoni <i>The mesophases of the α,ω-bis(4'-cyanobiphenyl-4-yl) undecane symmetric dimer</i></p>
<p>P51 – A. Bordogna, A. Pandini, <u>L. Bonati</u> <i>Predicting the accuracy of protein-ligand docking on homology models</i></p>
<p>P52 – <u>G. Graziano</u> <i>On the molecular origin of cold denaturation</i></p>
<p>P53 – N. Manghisi, C. Leggio, A. Jover, F. Mejjide, N. V. Pavel, V. H. Soto Tellini, J. Vázquez Tato, R. G. Agostino, <u>L. Galantini</u> <i>Catanionic Tubules with Tunable Charge</i></p>
<p>P54 – <u>M. C. Baratto</u>, A. Martorana, A. Sinicropi, C. Bernini, R. Pogni, R. Basosi <i>Spectroscopic characterization of 4-(methylamino)-benzoic acid, a small precursor for the synthesis of new dyes</i></p>
<p>P55 - <u>G. Gatti</u>, I. Braschi, M. Cossi, C. Bisio, L. Marchese <i>Methyl Tert-Butyl Ether Adsorption on High Silica Faujasite: an Experimental and Computational Model Study</i></p>
<p>P56 - C. Bisio, G. Paul, F. Carniato, <u>G. Gatti</u>, E. Boccaleri, L. Marchese <i>Physico-chemical investigation of CTA-Saponite clay</i></p>
<p>P57 - <u>U. Cosentino</u>, D. Pitea, G. Moro, G.A.A Saracino <i>Theoretical characterization of a new candidate as conditional MRI contrast agent for molecular imaging</i></p>
<p>P58 - <u>U. Cosentino</u>, D. Pitea, G. Moro, G.A.A. Saracino <i>Computational modelling of de novo synthesis of DibenzoFuran</i></p>

Sessione poster 2

Martedì 21 settembre 2010

14:00 – 15:15

<p>P59 – <u>A. Le Donne</u>, M. Acciarri, <u>S. Binetti</u> <i>Rare earth organic complexes as down-shifters to improve Si-based solar cell efficiency</i></p>
<p>P60 - <u>A. Benedetti</u>, I. Freris, P. Riello, F. Enrichi, D. Cristofori <i>Single Step Sol-Gel Synthesis of Luminescent Europium-Doped Zirconia Nanoparticles</i></p>
<p>P61 – L. Cavaciocchi, <u>F. Gambinossi</u>, P. Baglioni, G. Caminati <i>Layer-by-Layer solar cell based on a polymer/fullerene bulk heterojunction</i></p>
<p>P62 – <u>A. Painelli</u>, C. Sissa, L. Grisanti, F. Terenziani <i>Multibranching CT chromophores in solution: symmetry-breaking and beyond</i></p>
<p>P63 - <u>M. R. Martina</u>, T. Al Kayal, F. Z. Sadafi, D. Berti, G. Caminati <i>Models for Lipid Raft: A Study in Synthetic Lipid Vesicles</i></p>
<p>P64 - <u>A. E. Di Mauro</u>, R. Comparelli, E. Fanizza, N. Depalo, M. Striccoli, A. Agostiano, M. L. Curri <i>2/3D organization of CdS nanocrystals: towards innovative functional materials</i></p>
<p>P65 – <u>A. Schiraldi</u>, P. Pani, M. Signorelli, D. Fessas <i>Thermodynamic Approach to Osmo-Dehydration</i></p>
<p>P66 – P. Carniti, <u>A. Gervasini</u>, M. Marzo <i>Intrinsic vs. effective acidity of solid catalysts in water and polar liquids</i></p>
<p>P67 – <u>A. Gervasini</u>, M. Marzo <i>On the activity of mixed oxides towards VOC oxidation studied by a thermal gravimetric method</i></p>
<p>P68 - <u>F. Bellissima</u>, F. Carta, A. Innocenti, C. Supuran, A. Scozzafava, D. Berti, P. Baglioni <i>Gold nanoparticles Coated with a Carbonic Anhydrase Inhibitor: Size and Functionalization Control</i></p>
<p>P69 - C. Milanese, A. Girella, G. Bruni, V. Berbenni, A. Colella, A. Bianchin, P. Matteazzi, <u>A. Marini</u> <i>The “Nanostore” project: development of an innovative Mg – based material for solid state hydrogen storage</i></p>
<p>P70 - <u>D. Meroni</u>, G. Cappelletti, R. Annunziata, M. Benaglia, S. Rossi, M. Ratti, S. Ardizzone <i>The nature of the hydrophobic layer in hybrid nanomaterials</i></p>

<p>P71 – D. Meroni, V. Pifferi, F. Spadavecchia, M. Vescovi, I. Biraghi <i>Tailored TiO₂ nanoparticles by means of template and microemulsion routes</i></p>
<p>P72 – C. Oliva, F. Spadavecchia, D. Meroni, G. Cappelletti, S. Ardizzone, S. Cappelli <i>EPR features of second generation photocatalysts</i></p>
<p>P73 – A. Ferrarini, A. Marini, B. Mennucci <i>From electronic structure to liquid crystal properties: a coupled computational strategy for bent-core mesogens</i></p>
<p>P74 – D. Bressanini, M. Carboni, G. Morosi <i>A diffusion Monte Carlo simulation of BeN linear chains</i></p>
<p>P75 – A. Panniello, R. Comparelli, M. L. Curri, A. Agostiano, R. Tommasi, M. Striccoli <i>Nanocrystal based luminescent nanocomposites: effect of synthetic parameters and chemical environment on the recombination dynamics</i></p>
<p>P76 – E. Carretti, E. Fratini, D. Berti, L. Dei, P. Baglioni <i>Nanoscience for Art Conservation: Oil-in-Water Microemulsions Embedded in a Polymeric Network for the Cleaning of Works of Art</i></p>
<p>P77 – L. Varriale, N. Tonge, N. Bhalla, A. M. Ellis <i>Near-Infrared spectroscopy of mass-selected Li(NH₃)_n and Li(ND₃)_n clusters: observation of solvated electron transition</i></p>
<p>P78 – L. Varriale, N. Tonge, N. Bhalla, A. M. Ellis <i>Vibrational and electronic transitions of metal-solvent clusters</i></p>
<p>P79 – D. Capsoni, M. Bini, S. Ferrari, P. Mustarelli, V. Massarotti, M. C. Mozzati, A. Spinella <i>The role of Mn doping in LiTi₂(PO₄)₃ material for lithium batteries</i></p>
<p>P80 – M. A. Budroni, F. Rossi, M. Masia, N. Marchettini, M. L. T. Liveri, M. Rustici <i>Origin and extinction of chaotic oscillations in the Belousov-Zhabotinsky reaction</i></p>
<p>P81 – F. Rossi, V. Vanag, I. Epstein, E. Tiezzi <i>Cross-Diffusion and pattern formation in multi-component systems</i></p>
<p>P82 – A. De Bonis, J. V. Rau, A. Santagata, A. Galasso, L. Maio, R. Teghil <i>Ultra-short Pulsed Laser Deposition of super-hard thin films of transition metal borides</i></p>
<p>P83 – M. V. Dozzi, B. Ohtani, E. Selli <i>Effects of fluorine doping on the photocatalytic activity of TiO₂ in liquid and gas phase reactions</i></p>

<p>P84 – N. Peruzzi, <u>P. Lo Nostro</u>, M. Severi, B. W. Ninham, P. Baglioni <i>A Phase Separated System can act as a Chemical Sponge: Asymmetric Partitioning of Anions in Lysozyme Dispersions</i></p>
<p>P85 – <u>P. Lo Nostro</u>, L. Tattini, M. Bonini, P. Baglioni <i>PZT Nanoparticles for Piezoelectric Devices</i></p>
<p>P86 – C. Musumeci, A. Luzio, M. H. Rosnes, C. P. Pradeep, H. N. Miras, L. Cronin, <u>B. Pignataro</u> <i>Physical processes and chemical properties guiding polyoxometalates self-structuring on surfaces</i></p>
<p>P87 – A. Luzio, C. Musumeci, C. R. Newman, A. Facchetti, T. J. Marks, <u>B. Pignataro</u> <i>On the achievement of high performance organic thin film transistors by solution processes</i></p>
<p>P88 - G. Arrabito, <u>B. Pignataro</u> <i>Inkjet printing arrays and their application for drug screening</i></p>
<p>P89 - G. Pizzorusso, M. Neubauer, <u>E. Fratini</u>, R. Giorgi and P. Baglioni <i>Chemical gels for the cleaning of easel paintings</i></p>
<p>P90 – <u>G. Giancane</u>, S. Bettini, G. M. Farinola, C. Martinelli, A. Santino, L. Valli <i>Immobilization and stabilization of natural anthocyanins and innovative applications</i></p>
<p>P91 - <u>P. D'Angelo</u>, R. Caminiti <i>Local structure of ionic liquids probed by EXAFS</i></p>
<p>P92 - G. Malavasi, A. Pedone, A. J. Salinas, M. Vallet-Regí, <u>M.C. Menziani</u> <i>The bioactivity of SiO₂-CaO and SiO₂-CaO-P₂O₅ sol-gel glasses explained by molecular dynamics simulations</i></p>
<p>P93 – M. Del Cadia, A. Barbosa, F. De Rienzo, <u>M. C. Menziani</u> <i>The ligand recognition sites of homo- and heteropentameric 5-HT₃ Receptors from a computational point of view</i></p>
<p>P94 - C. Artini, <u>G. A. Costa</u>, R. Masini <i>Phase stability study of the pseudobinary system Gd₂O₂CO₃-Nd₂O₂CO₃ (420°C ≤ T ≤ 660°C)</i></p>
<p>P95 - A. Borsese, M. M. Carnasciali, <u>G. A. Costa</u> <i>The melting heat is “latent”?</i></p>
<p>P96 - K. F. Pirker, <u>M. C. Baratto</u>, R. Basosi, B. A. Goodman <i>Multifrequency EPR study of GA- and EGCG-Cu(II) complexes</i></p>
<p>P97 – C. Montis, S. Milani, P. Baglioni, <u>D. Berti</u> <i>Interaction of Nucleolipoplexes with Giant Vesicles as Cell Membrane Models. A Confocal Microscopy study</i></p>

<p>P98 – <u>B. Carlotti, F. Elisei</u> <i>Fast and ultrafast spectroscopic investigation of tetracyclines and their complexes with metal ions and DNA</i></p>
<p>P99 – <u>M. Battezzati, V. Magnasco</u> <i>Interaction energy of coupled permanent dipoles in oriented molecules</i></p>
<p>P100 - <u>C. A Guido, B. Mennucci, D. Jacquemin, C. Adamo</u> <i>Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory</i></p>
<p>P101 – <u>G. L. Chiarello, A. Di Paola, L. Palmisano, M. Pedroni, E. Selli</u> <i>Photocatalytic performance of brookite in hydrogen production by photo-steam reforming</i></p>
<p>P102 – <u>A. Saccomanni, M. V. Dozzi, E. Selli</u> <i>Photocatalytic Activity of F-doped TiO₂ Modified by Noble Metal Nanoparticles Deposition</i></p>
<p>P103 - <u>A. Costantino, L. Simeone, G. Mangiapia, D. Montesarchio, G. D’errico, O. Ortona, R. Sartorio, L. Paduano</u> <i>A new class of potential antineoplastic agents based on ruthenium amphiphilic nanostructures</i></p>
<p>P104 – <u>G. Vitiello, A. Merlino, F. Sica, E. Busi, R. Basosi, L. Paduano, G. D’Errico</u> <i>A combined experimental and molecular dynamics simulation study on the interaction between a peptide deriving from glycoprotein gp36 of feline immunodeficiency virus and phospholipid membranes</i></p>
<p>P105 – <u>C. Gatti</u> <i>The Source Function descriptor as a tool to extract chemical information from theoretical and experimental electron densities</i></p>
<p>P106 – <u>G. Alberto, G. Viscardi, G. Caputo, S. Coluccia, G. Martra</u> <i>Hybrid Fluorescent Dyes-Silica Nanoparticles: Toward a Possible Molecular Control of the Photophysical Properties</i></p>
<p>P107 – <u>M. Argeri, A. Fraccarollo, F. Grassi, L. Marchese, M. Cossi</u> <i>Theoretical modeling of PbSe nanoclusters: effect of surface passivation on shape and composition</i></p>
<p>P108 – <u>A. Biancardi, A. Marini, A. Muñoz-Losa, B. Mennucci</u> <i>Photophysical properties of environment-sensitive fluorescent probes by means of DFT calculations</i></p>
<p>P109 – <u>F. Olivero, F. Carniato, L. Marchese</u> <i>A novel bifunctional Polyhedral Oligomeric Silsesquioxane bearing in the structure luminescent and drug entities. A molecular platform for biomedical applications</i></p>

<p>P110 – <u>A. Pedone</u>, J. Bloino, S. Monti, G. Prampolini, V. Barone <i>Absorption and Emission Spectra of Fluorophores encapsulated in Silica nanoparticles: a QM/MM/PCM Study</i></p>
<p>P111 - V. Barone, I. Cacelli, A. Ferretti, S. Monti, <u>G. Prampolini</u> <i>Accurate and reliable calculation of magnetic interaction in organic diradicals</i></p>
<p>P112 – <u>E. Piccinelli</u>, E. Collina, M. Lasagni, A. Pirovano, D. Pitea <i>A reaction mechanism of native carbon thermal degradation and PCDD/F formation on MSWI fly as</i></p>
<p>P113 - <u>F. Cucinotta</u>, F. Carniato, G. Paul, S. Caldarelli, L. Marchese <i>Incorporation of Super Yellow polymer into mesoporous SBA-15 platelets: towards new luminescent hybrid systems</i></p>
<p>P114 – <u>M. Pavone</u>, M. Biczysko, N. Rega, V. Barone <i>Magnetic properties of nitroxide spin-probes: reliable account of molecular motions and non specific solvent effects by time-dependent and time-independent approaches</i></p>
<p>P115 – <u>E. Stendardo</u>, A. Pedone, P. Cimino, M. C. Menziani, O. Crescenzi, V. Barone <i>Extension of the AMBER force-field for the study of large nitroxides in condensed phases: an ab initio parameterization</i></p>
<p>P116 – <u>N. Rega</u>, G. Brancato, V. Barone <i>Stokes shift dynamics of a solvatochromic dye: simulation and analysis</i></p>

